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## Modelling of the electrical resistivity of ferromagnetic and paramagnetic intermetallic compounds

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**Abstract.** The temperature dependence of the electrical resistivity of some magnetic intermetallic compounds is analysed using a model which takes into account the changes in the electronic structure with the variation of the long-range order, neglecting chemical and magnetic short-range order (SRO) effects. The values of atomic and magnetic long-range order (LRO) parameters are obtained using a magnetic-cluster variation method (CVM) approach with the interaction parameters fitted to the equilibrium phase diagrams. The three principal components of the resistivity, namely the chemical disorder, the magnetic disorder, and the electron-phonon scattering contributions, are reproduced well for several paramagnetic (NiPt,  $\text{Fe}_{0.7}\text{Al}_{0.3}$ ) and ferromagnetic (CoPt,  $\text{Co}_{0.3}\text{Pt}_{0.7}$ ) compounds. Our analysis indicates an important change in the electronic structure with the variation of the LRO parameter, this effect being very pronounced in  $\text{Fe}_{0.7}\text{Al}_{0.3}$ .

### 1. Introduction

Resistivity measurement, despite its declining utilization, remains a powerful tool for the investigation of microstructural and physical phenomena in metallic systems. The technique is particularly useful for the study of defects such as vacancies and of their mobility, studies of phase separation phenomena and determination of phase diagram limits, i.e. of critical transformation concentrations and/or temperatures. Furthermore, resistivity can be measured at high temperatures and over long time periods with a very large accuracy, thus being well adapted for the investigation of kinetics and of correlated processes, such as ordering and disordering phenomena. For example, recent resistivity measurements coupled with *in situ* TEM experiments in an ordered  $L1_2$  CoPt<sub>3</sub> compound [1] have shown that the antiphase boundaries separating different ordered domains are progressively wetted by the disordered phase when approaching the critical order-disorder transition from below. The resistivity, and more precisely its temperature derivative and its time dependence, allowed the authors to distinguish the temperature range where the disorder appears along the antiphase boundaries from the temperature range where the disordered phase nucleates inside the ordered domains [1].

From a more fundamental viewpoint, the problem of understanding the behaviour of the resistivity in terms of changes in the electronic structures of compounds is of considerable general interest. In particular, one would like to understand why the resistivity increases or decreases in the vicinity of the order-disorder phase transitions.

The answer to this question is not trivial. An up-to-date and comprehensive book has been recently devoted by Rossiter [2] to the understanding of the resistivity of concentrated alloys and compounds. It is also the aim of the present paper to make a contribution to this problem.

The purpose of this work is to analyse our previous measurements of resistivity in several ordered compounds ( $L1_2$  Ni<sub>0.3</sub>Pt<sub>0.7</sub> and Co<sub>0.3</sub>Pt<sub>0.7</sub> [3],  $L1_0$  NiPt and CoPt [4] and  $DO_3$  and  $B2$  Fe<sub>1-C</sub>Al<sub>C</sub> [5]) through both their order-disorder transitions, and, for the ferromagnetic phases, their Curie temperatures. Our model follows the general approach developed by Rossiter [2] for the case of non-magnetic alloys. This model takes into account the changes in the electronic structure associated with the formation of long-range ordered phases. Here, the model is extended to the case of ferromagnets. Furthermore, we introduce reliable values of chemical (and magnetic) long-range order (LRO) parameters that are the intrinsic variables of the model. These LRO parameters, as a function of temperature,  $T$ , and concentration, are calculated from previous cluster variation method (CVM) (or magnetic CVM) simulations of the chemical and magnetic phase diagrams [6].

The paper is organized as follows. In section 2 we summarize our previous resistivity data [3–5] and their analysis using a statistical approach [7]. In section 3 we describe our new model and we present results in both non-magnetic (NiPt and Fe<sub>0.7</sub>Al<sub>0.3</sub>) and ferromagnetic (CoPt and Co<sub>0.3</sub>Pt<sub>0.7</sub>) compounds. The last section (4) is devoted to the discussion.

## 2. Previous results

Our previous investigations of the electrical resistivity in the intermetallic Co–Pt and Fe–Al compounds [3–5] have shown that the resistivity of these concentrated alloys can be written, to a first approximation, as the sum of either three or two contributions, in both ordered (O) and disordered (D) states, depending on whether or not the compounds display ferromagnetism at low temperatures:

$$\rho^{\text{tot } \alpha(D)}(T) = \rho_0^{\alpha(D)} + \mathcal{A}^{\alpha(D)}T + \rho_m^{\alpha(D)}. \quad (1)$$

$\rho_0^{\alpha(D)}$  is the residual resistivity or atomic disorder term which depends on temperature in the LRO state through the variation of the LRO parameter ( $\eta$ ), and is nearly constant in the disordered state.  $\mathcal{A}^{\alpha(D)}T$  is the phonon term and its coefficient  $\mathcal{A}$  is also dependent of temperature through  $\eta$ . The third term  $\rho_m^{\alpha(D)}$  is the spin disorder scattering term which is zero at low temperature in a ferromagnetic phase, and is negligible at any temperature in non-magnetic phases. In a simple localized spin model as described in [9, 10]  $\rho_m$  is expected to increase from zero at low temperature to its maximum value at the Curie temperature  $T_{\text{CM}}$ , and to remain constant in the paramagnetic state.

All resistivity measurements were carried out on samples that have attained thermodynamic equilibrium, when allowed by diffusion rates at each temperature, i.e. above 700–800 K in Ni–Pt and Co–Pt phases, and above about 600 K in Fe–Al.

### 2.1. Non-magnetic alloys

Since in Ni–Pt and Fe–Al alloys the magnetic contribution  $\rho_m$  is zero, it is relatively simple to separate the contribution of the chemical disorder from that of the electron-phonon scattering. In addition to the total resistivity, the residual resistivity due to

the chemical disorder,  $\rho_0^{\text{O(D)}}$ , was measured by quenching the sample rapidly to 4 K from an equilibrium state at high temperature characterized by a LRO parameter,  $\eta$ . The phonon contribution is given by the difference:

$$\rho_{\text{ph}} = \mathcal{A}^{\text{O(D)}} T = \rho^{\text{tot}}(T) - \rho_0^{\text{O(D)}} [\eta(T)].$$

The results obtained for Ni-Pt and for some  $\text{Fe}_{1-C}\text{Al}_C$  alloys having either the  $\text{DO}_3$  or the  $B2$  structure are shown in figures 1 and 2. Figures 1 and 2 display the measured total and residual resistivities, and the phonon contribution deduced from their difference. In general one observes the expected increase of  $\rho_0$  when  $\eta$  decreases, whereas the phonon coefficient  $\mathcal{A}$  remains constant as long as  $\eta$  is constant, and decreases when  $\eta$  decreases. This effect is more pronounced in NiPt,  $\text{Fe}_{0.7}\text{Al}_{0.3}$  and  $\text{Fe}_{0.67}\text{Al}_{0.33}$ . In other  $\text{Fe}_{1-C}\text{Al}_C$  alloys, which have the  $B2$  structure ( $C = 0.40$  and  $0.45$ ), the variation of  $\rho_{4\text{K}}$  with  $T$  is very small. This is due to the fact that, above about 850 K, the quenching rate is not sufficiently rapid to freeze in the high- $T$  equilibrium states. This point is illustrated in figure 3 where the values of  $\rho_{4\text{K}}$  in both the ordered and the disordered states are compared. Above 36% of Al, we do not observe any difference in the residual resistivities of ordered and quenched samples.

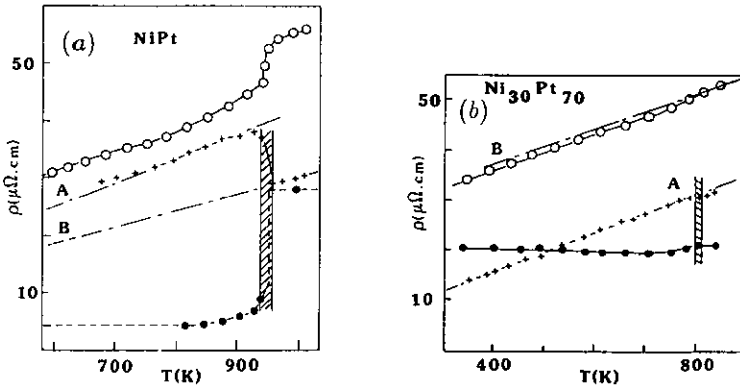


Figure 1. Resistivity data from [3, 4] in NiPt (a) and  $\text{Ni}_{0.3}\text{Pt}_{0.7}$  (b). Total (O), residual (●) and phonon (+) resistivities. The dot-dashed lines are least-squares fits of  $\rho_{\text{ph}}^{\text{O}} = \mathcal{A}^{\text{O}} T$  (line A) and  $\rho_{\text{ph}}^{\text{D}} = \rho_0^{\text{D}} + \mathcal{A}^{\text{D}} T$  (line B).

By measuring the values of the phonon coefficient  $\mathcal{A}$  for various concentrations over the low temperature range, where the lack of diffusion freezes  $\eta$  to a constant value ( $\eta_{T \rightarrow 0} = \eta_{\text{max}}$ ), it is possible to observe the great sensitivity of  $\mathcal{A}(T \rightarrow 0)$  to the disorder due to off-stoichiometry defects, as shown in figure 4. It is clear from figures 2 and 4 that  $\mathcal{A}$  is maximum at low  $T$  for the stoichiometric compositions and is minimum either in the disordered state (figure 2) or the largest off-stoichiometry (figure 4).

These results in non-magnetic Ni-Pt and Fe-Al alloys show that the phonon contribution is strongly correlated to the degree of order.

## 2.2. Ferromagnetic alloys

Since for ferromagnetic alloys there are three contributions to the resistivity and only two experimental determinations, it was necessary to make some hypotheses

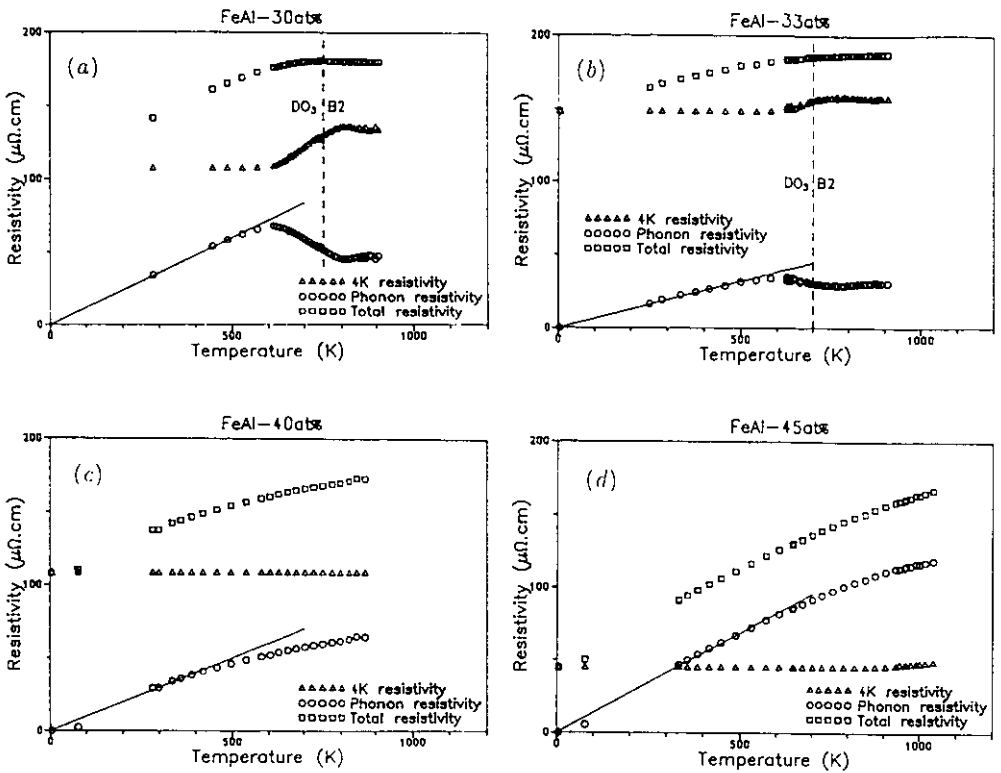


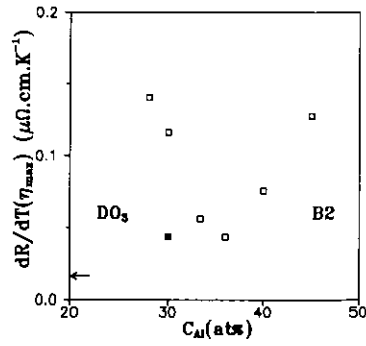
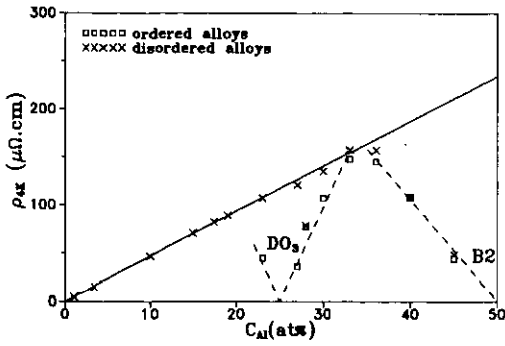
Figure 2. Resistivity results in  $\text{Fe}_{1-C}\text{Al}_C$  alloys for  $C = 0.3$  (a),  $0.33$  (b),  $0.40$  (c),  $0.45$  (d). The dotted line indicates the  $\text{DO}_3\text{-B2}$  transition, the full line, the slope of the phonon term ( $\mathcal{A}$ ) in the LRO state when  $\eta$  is constant.

in order to separate the various terms in equation (1). In view of the similarities between the vibrational properties of Co-Pt and Ni-Pt phases [3, 4], we first assumed that the phonon coefficients  $\mathcal{A}$  are the same in both Co-Pt and Ni-Pt phases for a given composition and structure. So, using reduced temperature scales  $T/T_{\text{OD}}$ , it was possible to transfer the values of  $\mathcal{A}(\eta(T/T_{\text{OD}}))$  determined in the  $\text{Ni}_{1-C}\text{Pt}_C$  compounds to the  $\text{Co}_{1-C}\text{Pt}_C$  compounds, and then to get  $\rho_m(T)$  from equation (1).

The values obtained for  $\rho_m$  in CoPt and  $\text{Co}_{0.3}\text{Pt}_{0.7}$  are compared to the measured residual resistivity values in figure 5. One observes the expected increase of  $\rho_m$  up to  $T_{\text{CM}}$  in the two phases, and an unexpected decrease in the paramagnetic range over the  $T$ -range where  $\eta$  decreases. For  $\text{Co}_{0.3}\text{Pt}_{0.7}$ , the decrease of  $\rho_m$  around  $T_{\text{OD}}$  would be overestimated due to a bigger uncertainty in the evaluation of the phonon contribution.

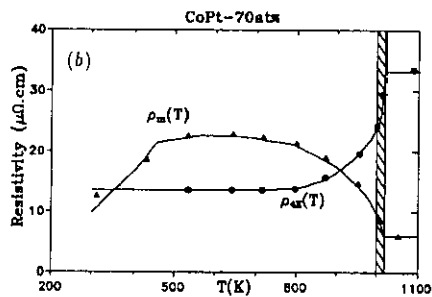
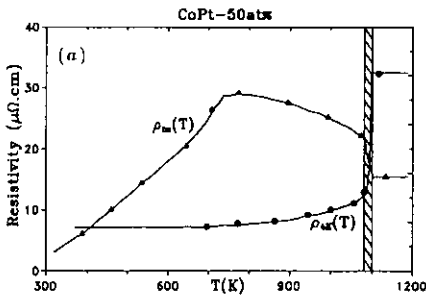
Nevertheless, these results show that, in the paramagnetic range, the spin disorder scattering term, as well as the phonon contribution, is strongly dependent on the degree of order.

In order to understand the origin of the decrease of  $\rho_m$  at the order-disorder transition, we first proposed in [3, 4] a qualitative interpretation in terms of a localized magnetism model in which the short-range magnetic correlations in the paramagnetic state would be enhanced by the chemical disorder. A purely statistical CVM approach, where the atomic and spin disorder contributions to the resistivity



**Figure 3.** Residual resistivity as a function of  $C$  in  $Fe_{1-C}Al_C$  alloys. The crosses correspond to disordered alloys rapidly quenched from about  $1000^\circ\text{C}$ , a temperature which corresponds to the solid solution phase up to 30% Al, and to the  $B2$  structure above. The squares correspond to the annealed ordered phases, in their highest order degree as allowed by diffusion. The dashed lines visualize the effects of departures from stoichiometry in the  $DO_3$  and  $B2$  phases.

**Figure 4.** Concentration dependence of the linear phonon coefficient ( $A$ ) as given by the slope of straight lines in figure 2. The full square is the value in the disordered state as deduced from the simulation of data. The arrow indicates the value in the disordered alloys for  $C \leq 0.2$ .



**Figure 5.** Resistivity data from [3, 4] in  $CoPt$  (a) and  $Co_{0.3}Pt_{0.7}$  (b); ● measured residual resistivity, ▲ estimated magnetic contribution as described in the text. The hatched area indicates the  $O-D$  transformation  $T$ -range.

were described as sums of resistivities of individual tetrahedral clusters, was then used [7]. In spite of a relative agreement between theory and experiment, such a purely statistical model, which contains severe approximations, is not able to reproduce the overall resistivity. Moreover, as mentioned in [7], the statistical approach neglects the changes in the electronic structure associated with the formation of the ordered structures. Therefore, in section 3 we propose a unified model where both the results of the CVM and the changes in the electronic structure are taken into account.

### 3. Resistivity analysis

#### 3.1. Model

Approximately ten years ago, Rossiter [2, 8] developed a theoretical approach aimed at the description of the overall dependence of the resistivity on the LRO parameter,  $\eta$ , in non-magnetic alloys. In the case of a stoichiometric compound and above the Debye temperature  $\theta_D$ , the resistivity is given by:

$$\rho(\eta, T) = \frac{\rho_0^D (1 - \eta^2(T))}{(1 - A\eta^2(T))} + \frac{BT}{n_0(1 - A\eta^2(T))} \quad (2)$$

where  $T$  is the temperature, and  $\rho_0^D$ ,  $n_0$  and  $B/n_0$  are, respectively, the residual resistivity, the density of conduction electrons, and the temperature coefficient of the phonon contribution in the disordered state.

Equation (2) was obtained by considering the effects of LRO on: (i) the scattering of the conduction electrons, and (ii) related changes in the electronic band structure.

The effect of long-range atomic ordering on the scattering of the conduction electrons is treated in an appropriate pseudo-potential model in the Bragg-Williams approximation. The resistivity is described within the simple relaxation time approximation in a nearly free electron model,

$$\rho = (m^*/n_{\text{eff}})/e^2\tau \quad (3)$$

where  $\tau$  is order dependent through:

$$\tau^{-1} = \tau_0^{-1} [1 - \eta^2(T)]. \quad (4)$$

$\tau_0$  is the relaxation time corresponding to the disordered state,  $m^*$  and  $n_{\text{eff}}$  are, respectively, the effective mass and the effective density of conduction electrons per unit volume.

Since the long-range atomic ordering may introduce new gaps into the Fermi surface at the superlattice Brillouin zone boundaries, Rossiter has shown that the value of  $n_{\text{eff}}$  (or  $n_{\text{eff}}/m^*$ ) will be order dependent according to the following expression:

$$n_{\text{eff}} = n_0 [1 - A\eta^2(T)]. \quad (5)$$

The coefficient  $A$  depends upon the relative positions of the Fermi surface and the superlattice Brillouin zone boundaries. Its sign determines the evolution of the electronic band structure near the Fermi level with the formation of the LRO structure. Thus, for a given concentration in a non-magnetic LRO phase, equation (2) may be written as:

$$\rho^{\text{Total}} = \rho_0(\eta(T)) + AT \quad (6)$$

where  $\rho_0$  is the residual resistivity term which is  $T$ -dependent through  $\eta(T)$ , and  $AT$  is the phonon contribution whose coefficient  $A = B/n_0[1 - A\eta^2(T)]$  is also  $T$ -dependent through  $\eta$ . Since  $B$  in equation (2) depends on  $\theta_D$ , the Debye

temperature, the approach neglects a possible weak dependence of  $\theta_D$  on  $\eta$ . This model has been already applied by Rossiter [8] to the cases of  $\text{Cu}_3\text{Au}$  and  $\text{Fe}_3\text{Al}$ .

We extend equation (2) to the case of ferromagnetic compounds by adding the term of spin disorder scattering. In the simple model of well defined local moments in a simple conduction band, as developed by Kasuya [9], De Gennes and Friedel [10], one can write  $\rho_m$  as:

$$\rho_m = \rho_m^P [1 - \sigma^2(T)] \tag{7}$$

where  $\sigma$  is the ferromagnetic LRO parameter being equal to 1 at  $T = 0$  and 0 at  $T_{CM}$ .  $\rho_m^P$  is the value of  $\rho_m$  in the paramagnetic state:

$$\rho_m^P = \text{constant} \times \mathcal{J}^2 / n_{\text{eff}} \tag{8}$$

where  $\mathcal{J}$  is the scalar value of the saturation moment yielding:

$$\rho_m = \rho_m^D [1 - \sigma^2(T)] / [1 - A\eta^2(T)] \tag{9}$$

$\rho_m^D$  being the value of  $\rho_m^P$  above  $T_{OD}$ .

### 3.2. Method of analysis

In order to test the model presented in the previous section, we first need to define and to know the LRO parameters and their  $T$ -dependence in the various structures. The values of the chemical and ferromagnetic LRO parameters,  $\eta(T)$  and  $\sigma(T)$ , are entered in equations (1), (2) and (7), and the remaining parameters are adjusted in order to reproduce the experimental results.

3.2.1. Determination of LRO parameters. The  $L1_2$ ,  $L1_0$ ,  $DO_3$  and  $B2$  structures are represented in figure 6.

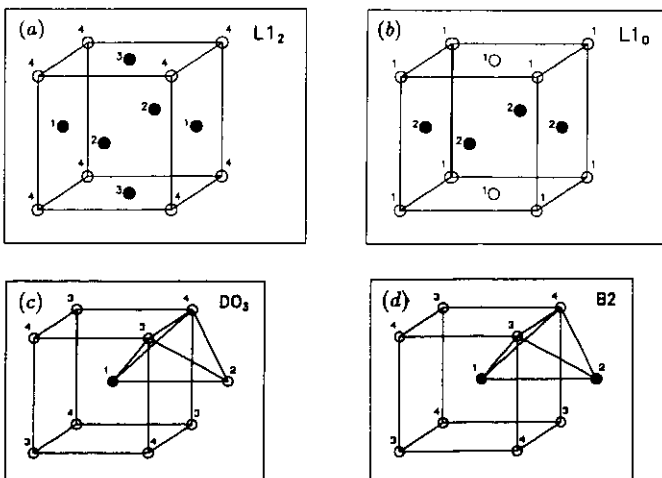


Figure 6.  $L1_2$ ,  $L1_0$ ,  $DO_3$  and  $B2$  structures.



**Chemical LRO.** The order state of the  $L1_2$  and  $L1_0$  phases is determined by a single order parameter  $\eta$ . If  $\langle P_A^i \rangle$  is the occupation probability of the  $i$  sublattice by an  $A$  atom and  $C_A$  the  $A$  concentration, one has in the  $L1_2$  ( $A_3B$ ) structure, which consists of four interpenetrating sublattices, three of them (1, 2, 3) being equivalent:

$$\eta = (\langle P_A^{1,2,3} \rangle - C_A) / (1 - \frac{3}{4}) \quad \text{for } 1 \geq C_A \geq 0.75$$

or

$$\eta = (\langle P_B^4 \rangle - C_B) / (1 - \frac{1}{4}) \quad \text{for } 1 \geq C_B \geq 0.25.$$

In the  $L1_0$  ( $AB$ ) structure, which consists of two inequivalent sublattices (1 and 2), one has:

$$\eta = (\langle P_{A(B)}^{1(2)} \rangle - C_{A(B)}) / (1 - \frac{1}{2}) \quad \text{for } C_{A(B)} \geq 0.5.$$

These simple expressions yield the maximum value of the order parameter at  $T = 0$  ( $\langle P_A^i \rangle_{T=0} = 1$ ) according to the concentration. One has:

$$\eta_{\max} = \begin{cases} 0.933 & \text{in } M_{0.3}Pt_{0.7} \\ 1 & \text{in MPt.} \end{cases}$$

In the  $DO_3$  structure, which consists of four interpenetrating sublattices with two of them (3 and 4) being equivalent, the order state is determined by two LRO parameters:

$$\left. \begin{aligned} \eta_1 &= \frac{1}{2} [\langle P_A^1 \rangle - \langle P_A^2 \rangle] \\ \eta_2 &= \frac{1}{2} [\langle P_A^1 \rangle + \langle P_A^2 \rangle - 2\langle P_A^3 \rangle] \end{aligned} \right\} \quad \text{for } C_A \geq 0.25 \quad (A = Al)$$

with the same definition as before.

In the  $B2$  structure, the sublattices 1 and 2 are equivalent ( $\eta_1 = 0$ ), and one has a single order parameter:

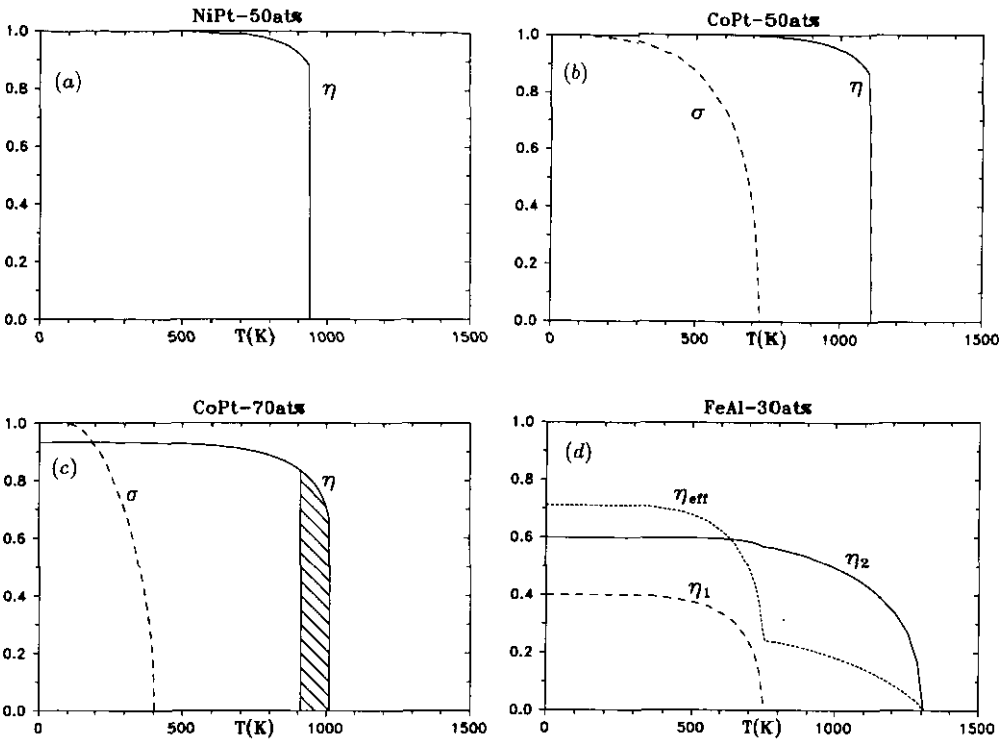
$$\eta = \eta_2 = \langle P_A^{1,2} \rangle - \langle P_A^{3,4} \rangle \quad \text{for } C_A \leq 0.5.$$

For  $Fe_{0.7}Al_{0.3}$ , the maximum values of the order parameters at  $T = 0$  are:

$$\begin{aligned} \eta_1 &= 0.4, \eta_2 = 0.6 && \text{in } DO_3 \\ \eta &= 0.6 && \text{in } B2. \end{aligned}$$

These single-site occupation probabilities are obtained by fitting the Ni-Pt and Co-Pt phase diagrams to experimental values using the tetrahedron approximation of a magnetic-CVM model with nearest-neighbour (NN) interactions only as described in [6]. In the case of  $Fe_{0.7}Al_{0.3}$ , the values of  $\eta_1$  and  $\eta_2$  were obtained by fitting the non-magnetic phase diagram to the experimental values of Afyouni [11], using the tetrahedron approximation of the CVM which, in a BCC lattice, includes NN and next-nearest-neighbour (NNN) interactions [12].

**Magnetic LRO.** The magnetic LRO parameter  $\sigma$  is defined as the expectation value of the spin operator at the site  $i$ ,  $S_i$ , which can take the values 0 or  $\pm 1$  according to whether site  $i$  is occupied, respectively, by a non-magnetic or by a magnetic atom. The  $T$ -dependences of calculated values of  $\eta$  and  $\sigma$  are shown in figure 7.



**Figure 7.** Temperature dependence of chemical and magnetic LRO parameters in the various structures,  $L1_0$  NiPt (a) and CoPt (b),  $L1_2$   $Co_{0.3}Pt_{0.7}$  (c),  $DO_3$  and  $B2$   $Fe_{0.7}Al_{0.3}$  (d). In (c), the hatched domain corresponds to the two-phase region. In (d),  $\eta_{eff}$  corresponding to equation (16) is plotted (dotted line) for the fitted value of  $D = 0.81$ .

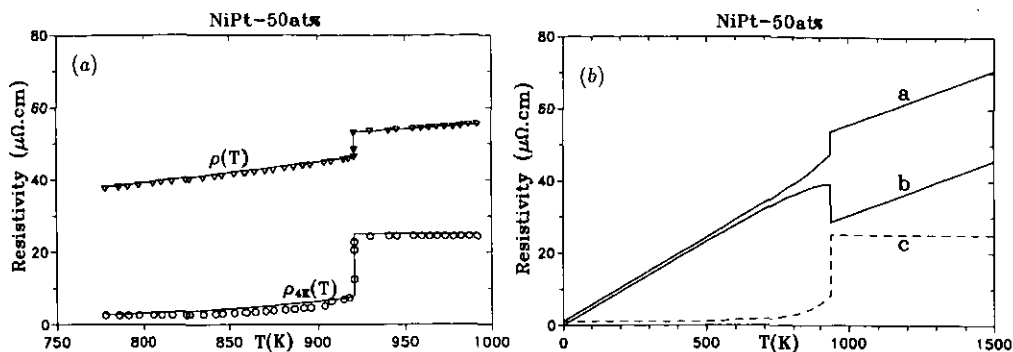
**3.2.2. Fit and simulation of the results.** Combining equations (1), (2) and (7) in a form tractable for the fit to the experimental results we have, in the general case, for all concentrations in the  $L1_2$  and  $L1_0$  phases:

$$\rho(T) = \rho_{APB} + \rho_0^D \left( 1 - \frac{C_A C_B}{\nu(1-\nu)} \eta^2(T) \right) / [1 - A\eta^2(T)] + \frac{B}{n_0} T / [1 - A\eta^2(T)] + \rho_m^D [1 - \sigma^2(T)] / [1 - A\eta^2(T)]. \tag{10}$$

The constant  $\rho_{APB}$  has been added to account for the presence of order defects, like antiphase boundaries, which are always present in the totally ordered compound at  $T = 0$  when  $\eta = 1$ . So, the total value of the residual resistivity in the disordered state is  $\rho_{APB} + \rho_0^D$ .

In the  $DO_3$  phase, which is described by two LRO parameters, the situation is more complicated. The changes of  $\eta_1$  and  $\eta_2$  do not affect the residual resistivity by the same quantity. In order to fit the experimental results, we define an effective LRO parameter by:

$$\eta_{eff} = \sqrt{\frac{16}{3} C_A C_B} \left( D\eta_1 + \sqrt{\frac{3}{4}} \eta_2 \right). \tag{11}$$



**Figure 8.** NiPt. (a) Comparison between experimental values of  $\rho_{4K}$  (O) and  $\rho_{\text{total}}$  ( $\nabla$ ) and the curves fitted through (10), over the  $T$  range of experiments. (b) Calculated values of  $\rho_{\text{total}}$  (a),  $\rho_{\text{phonon}}$  (b) and  $\rho_{4K}$  (c) between 0 and 1500 K.

Note that for the stoichiometric  $B2$  phase,  $\eta_{\text{eff}}$  reduces to  $\eta_2$ , as expected. The two series of experimental values of  $\rho$  ( $\rho_{4K}$  and  $\rho_{\text{total}}$ ) are least-squares fitted to relation (10) by adjusting the five variables  $\rho_{\text{APB}}$ ,  $\rho_0^D$ ,  $B/n_0$ ,  $\rho_m^D$  and  $A$  in the ferromagnetic Co-Pt phases, four variables ( $\rho_m^D = 0$ ) in the non-magnetic NiPt, and five variables (with  $D$ ) in  $\text{Fe}_{0.7}\text{Al}_{0.3}$ . At low temperatures, the values of  $\eta$  were kept constant and equal to their highest value allowed by diffusion. We did not fit  $\text{Ni}_{0.3}\text{Pt}_{0.7}$  since the variation of  $\eta$  in this compound, and thereby its effect on  $\rho$ , is very small.

The results of the fit are collected in table 1 and displayed in figures 8–11. In addition to the curves fitted to the experimental values, the calculated phonon and magnetic contributions are shown in figures 8(b)–11(b). On the whole the quality of the fits is satisfactory, showing the model works well in every case.

**Table 1.**

	$\rho_{\text{APB}}$ ( $\mu\Omega\text{ cm}$ )	$\rho_0^D$ ( $\mu\Omega\text{ cm}$ )	$B/n_0$ ( $\mu\Omega\text{ cm K}^{-1}$ )	$\rho_m^D$ ( $\mu\Omega\text{ cm}$ )	$A$
CoPt	6.65	23.44	0.0305	14.2	0.3776
$\text{Co}_{0.3}\text{Pt}_{0.7}$	10.17	21.55	0.0262	14.3	0.4236
NiPt	1.09	24.01	0.0305	0	0.343
$\text{Fe}_{0.7}\text{Al}_{0.3}$	0	140.4	0.0426	0	0.99

## 4. Discussion and conclusion

### 4.1. Chemical disorder term

Our approach assumes that  $\rho_{\text{APB}}$ , the contribution to the resistivity of lattice defects such as antiphase boundaries is temperature independent. Obviously  $\rho_{\text{APB}}$  also contributes to the total residual resistivity in the disordered state, which is given by the sum  $\rho_{\text{APB}} + \rho_0^D$ . The temperature independence of  $\rho_{\text{APB}}$  is indirectly confirmed by electron microscopy measurements which have shown that the width of antiphase

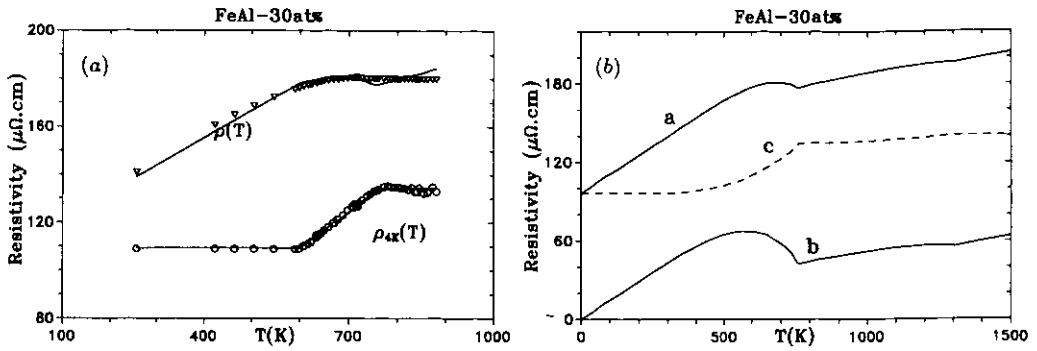


Figure 9. (a) As figure 8(a). (b) As figure 8(b). The change of the resistivity at the transition  $B2 \rightarrow A2$  is also shown.

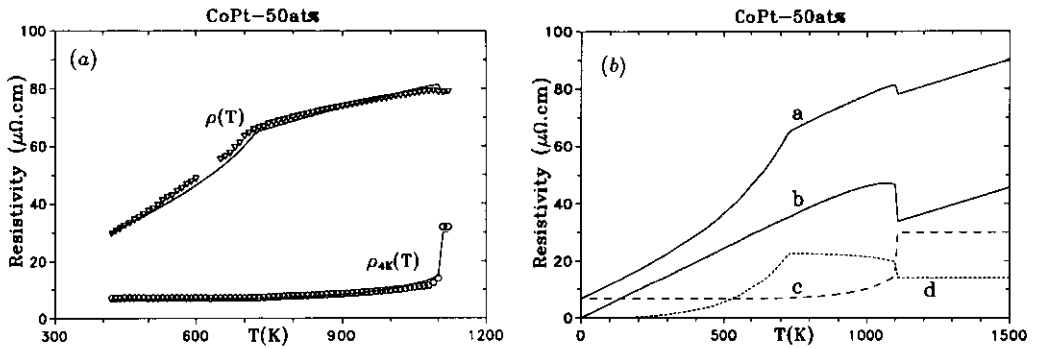


Figure 10. CoPt. (a) As figure 8(a). (b) As figure 8(b), with magnetic contribution (curve d).

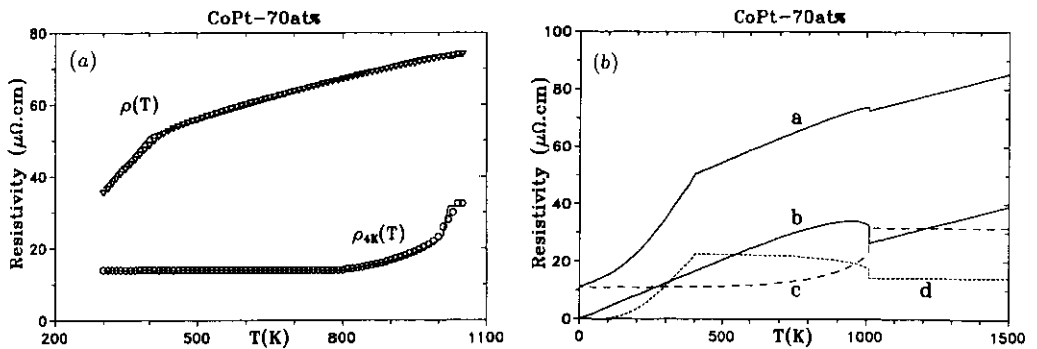


Figure 11.  $\text{Co}_{0.3}\text{Pt}_{0.7}$ , as figure 10.

boundaries remains constant up to about  $30^\circ\text{C}$  below  $T_{OD}$  [1]. Table 2 compares the fitted values of  $\rho_{APB}$  with the experimental values measured in stoichiometric phases (MPt,  $\text{MPt}_3$ ,  $\text{Fe}_3\text{Al}$ ) in their maximum degree of order. The agreement is quite good.

Table 2.

Alloy	$\rho_{\text{APB}}^{\text{fit}}$ ( $\mu\Omega$ cm)	$\rho_{\text{APB}}^{\text{experimental}}$ ( $\mu\Omega$ cm)	Reference
CoPt	6.6	5	[3]
Co <sub>0.3</sub> Pt <sub>0.7</sub>	10.2	12	[3]
NiPt	1.1	2	[3]
Fe <sub>0.7</sub> Al <sub>0.3</sub>	0	~0	Figure 3

The  $T$ -dependence of  $\rho_{4K}$  is well reproduced in the four samples. In Co<sub>0.3</sub>Pt<sub>0.7</sub>, there is a small disagreement at the vicinity of  $T_{\text{OD}}$  due to the presence of a two-phase region, over a range of about 10°C, which is not taken into account in our description.

In Fe<sub>0.7</sub>Al<sub>0.3</sub>, the fitted value of  $D$  is 0.81. We note that the calculated  $\rho_{\text{total}}(T)$  curve displays the behaviour observed by Afyouni [11] in Fe<sub>0.73</sub>Al<sub>0.27</sub> at the B2-A2 transition.

#### 4.2. Phonon term

The non-magnetic NiPt and Fe<sub>0.7</sub>Al<sub>0.3</sub> phases, for which the phonon contribution is uniquely determined from the two experimental measurements, provide a test of the approximations in the description of the phonon term by:

$$\rho_{\text{ph}} = \{ B / [n_0(1 - A\eta^2)] \} T.$$

Figures 8 and 9 show that the model works well. This agreement justifies the use of the above formulation for magnetic phases. Our analysis (table 1) yields similar values of  $B/n_0$  in NiPt and CoPt and a small difference in the values of  $A$ , justifying, *a posteriori*, the previous hypothesis (3), regarding the similarity of the phonon terms in these two phases. At  $T_{\text{OD}}$ , the phonon coefficient decreases in all the phases investigated, since  $A$  is found to be positive.

#### 4.3. Magnetic disorder term

In both CoPt and Co<sub>0.3</sub>Pt<sub>0.7</sub> the calculated magnetic terms display the same behaviour, being maximum at  $T_{\text{CM}}$ , and decreasing at  $T_{\text{OD}}$ , according to equation (9). In CoPt, comparison of the simulated curve with that deduced from experiment (figure 3) yields a satisfactory agreement, indicating that the formulation of  $\rho_{\text{m}}$  by equation (9) is correct to first approximation. The maximum values of  $\rho_{\text{m}}$  just above  $T_{\text{CM}}$  are about 22–23  $\mu\Omega$  cm in the two phases which, compared with the value estimated in nickel (20  $\mu\Omega$  cm) [13], is of the correct magnitude. In this model, the  $T$ -dependence of  $\rho_{\text{m}}$  in the paramagnetic state would be due mainly to the change in the electronic structure with  $\eta$ . The effect of atomic disordering on short-range magnetic correlations would be less important than we had initially thought [3, 4] and also than shown by statistical models [7].

#### 4.4. Discussion of $A$ and conclusion

First we note that our values of  $A$  compare well with other determinations made previously by Rossiter [2], who obtained  $A = 0.4$  for Cu<sub>3</sub>Au and 0.75 for Fe<sub>3</sub>Al.

This positive value of  $A$  means an increase in the effective number of conduction electrons in the disordered state compared to the ordered one, for all the ordered

Table 3.

	$n_{\text{eff}}^{\text{D}}/n_{\text{eff}}^{\text{O}}$		$\gamma^{\text{D}}/\gamma^{\text{O}}$	Reference
	$(\eta = 1)$	$(\eta = 0.9)$		
CoPt	1.61	1.44	1.33	[14]
NiPt	1.52	1.38	1.21	[14]
$\text{Co}_{0.3}\text{Pt}_{0.7}$	1.58		0.73	[14]
$\text{Fe}_{0.7}\text{Al}_{0.3}$	$\sim 8.5$		$> 1$	D [15] O [16] for $x_{\text{Al}} = 0.25$

structures  $L1_2$ ,  $L1_0$  and  $DO_3$ . Due to the very simplified formulation of the resistivity by equation (3), which is quite approximate for alloys of transition metals with high density of d electrons at the Fermi level, it is difficult to draw significant conclusions about the electronic structure changes induced by the formation of LRO phases. Comparison with other experiments, like measurements of the coefficient  $\gamma$  of the electronic specific heat, which yield information on the total density of states at the Fermi level, could be fruitful. Table 3 compares our ratio  $n_{\text{eff}}^{\text{D}}/n_{\text{eff}}^{\text{O}}$  given by  $1/(1-A)$  for several values of  $\eta$  with the ratio of  $\gamma^{\text{D}}/\gamma^{\text{O}}$ .

In NiPt and CoPt, our value of  $A$  indicates a decrease in the total density of states at the Fermi level in agreement with specific heat data. In Fe-Al, measurements of  $\gamma$  for  $C_{\text{Al}} = 0.25$  indicate an increase of  $\gamma$  when the disorder increases, i.e. when passing from the  $DO_3$  [15] to the  $B2$  structure [16]. The value in the totally disordered phase is not available. Thus, we only have an indication that  $\gamma^{\text{D}}$  is larger than  $\gamma^{\text{O}}$ , i.e. the same trend as in NiPt and CoPt. The case of  $\text{Co}_{0.3}\text{Pt}_{0.7}$  is different:  $\gamma$  does not show the same behaviour as resistivity. At this time we cannot explain this difference.

To conclude we have shown that the simple model initially developed by Rossiter for non-magnetic phases and extended by us to magnetic systems allows us first to describe the dependence of all the contributions to the resistivity with the degree of order and, furthermore, provides the basis for understanding the observed increase or decrease in the total resistivity at the order-disorder transition. The sign and the amplitude of the variation of  $\rho$  at  $T_{\text{OD}}$  depend mainly on the importance of electronic structure effects associated with the formation of the LRO structure.

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